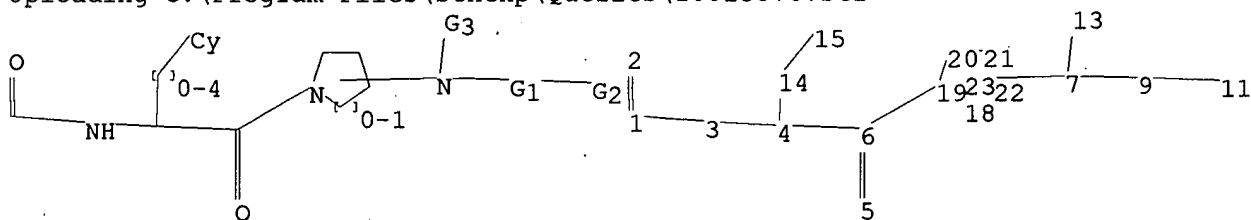


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chain nodes :

1 2 3 4 5 6 7 9 11 13 14 15

ring nodes :

18 19 20 21 22

chain bonds :

1-2 1-3 3-4 4-6 4-14 5-6 6-19 7-9 7-13 9-11 14-15

ring bonds :

18-19 18-22 19-20 20-21 21-22

exact/norm bonds :

1-2 1-3 3-4 5-6 6-19 7-9 7-13 9-11 14-15 18-19 19-20

exact bonds :

4-6 4-14 18-22 20-21 21-22

isolated ring systems :

containing 18 :

G1:C,S

G2: Cy,Ak

G3:Cb,Ak

Match level :

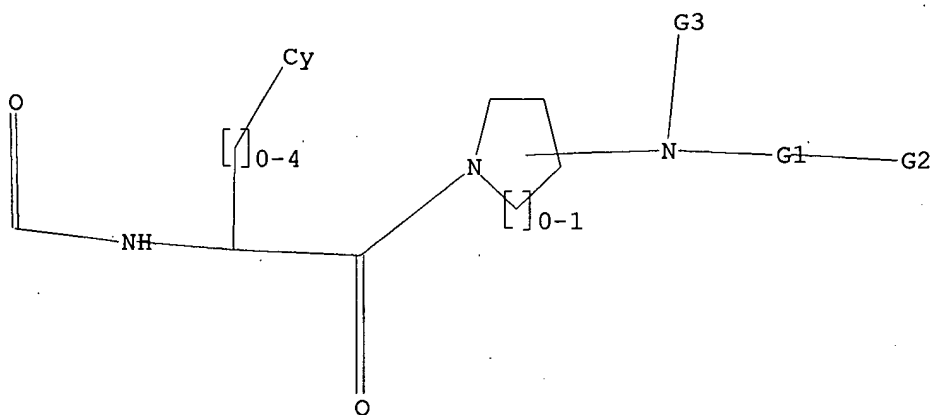
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13:CLASS 14:CLASS 15:Atom 18:Atom 19:Atom 20:Atom 21:Atom 22:Atom 23:CLASS

L1 STRUCTURE UPLOADED

=> dis l1

L1 HAS NO ANSWERS

L1 STR



G1 C,S

G2 Cy,Ak

G3 Cb,Ak

Structure attributes must be viewed using STN Express query preparation.

=&gt; s l1 sam

L2 3 SEA SSS SAM L1

=&gt; s l1 full

L3 207 SEA SSS FUL L1

=&gt; file caplus

=&gt; s l3

L4 5 L3

=&gt; s l4 and pd&lt;may 2003

23381835 PD&lt;MAY 2003

(PD&lt;20030500)

L5 2 L4 AND PD&lt;MAY 2003

=&gt; dis l5 1-2 bib abs hitstr

L5 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2005 ACS on STN

AN 2002:312325 CAPLUS

DN 137:47431

TI Novel Dipeptide Macrocycles from 4-Oxo, -Thio, and -Amino-Substituted Proline Derivatives

AU Arasappan, Ashok; Chen, Kevin X.; Njoroge, F. George; Parekh, Tejal N.; Girijavallabhan, Viyyoor

CS Schering Plough Research Institute, Kenilworth, NJ, 07033, USA

SO Journal of Organic Chemistry (2002), 67(11), 3923-3926

CODEN: JOCEAH; ISSN: 0022-3263

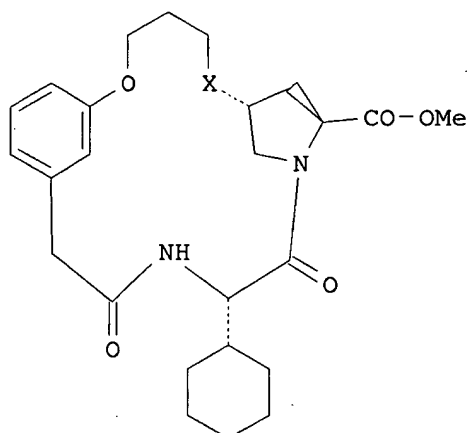
PB American Chemical Society

DT Journal

LA English

OS CASREACT 137:47431

GI



I

AB Dipeptide macrocycles [(I); X = O, S, N-SO<sub>2</sub>Ph] have been constructed in a versatile manner from the corresponding 4-heteroatom-substituted proline derivs. using an intramol. Mitsunobu strategy as the key step.

IT **367260-04-6P 367260-06-8P**

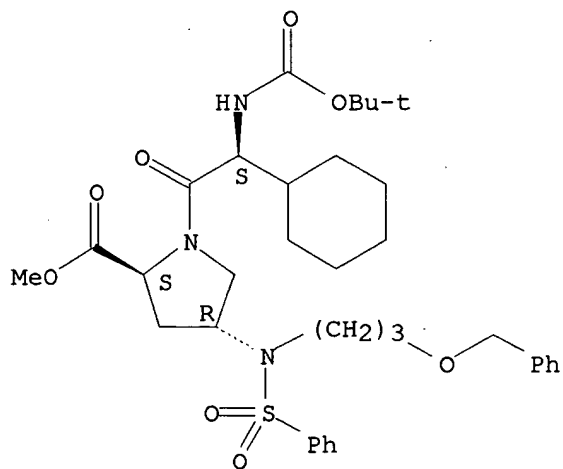
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of macrocyclic dipeptides via intramol. Mitsunobu cyclization)

RN 367260-04-6 CAPLUS

CN L-Proline, (2S)-2-cyclohexyl-N-[(1,1-dimethylethoxy)carbonyl]glycyl-4-[[3-(phenylmethoxy)propyl](phenylsulfonyl)amino]-, methyl ester, (4R)- (9CI)  
(CA INDEX NAME)

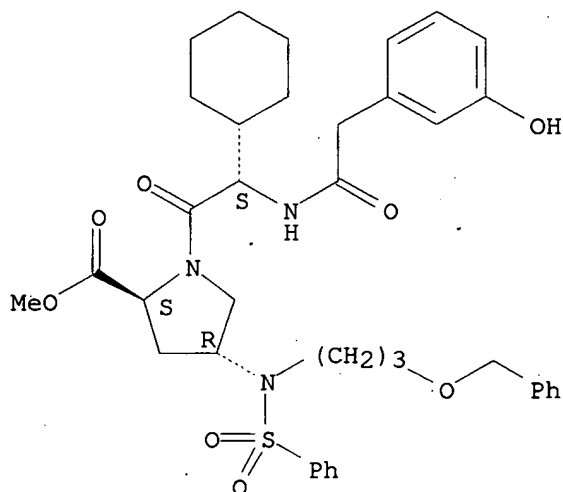
Absolute stereochemistry.



RN 367260-06-8 CAPLUS

CN L-Proline, (2S)-2-cyclohexyl-N-[(3-hydroxyphenyl)acetyl]glycyl-4-[[3-(phenylmethoxy)propyl](phenylsulfonyl)amino]-, methyl ester, (4R)- (9CI)  
(CA INDEX NAME)

Absolute stereochemistry.



RE.CNT 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2005 ACS on STN

AN 2001:763001 CAPLUS

DN 135:318715

TI Preparation of macrocyclic NS3-serine protease inhibitors of hepatitis C virus comprising n-cyclic p2 moieties

IN Chen, Kevin X.; Arasappan, Ashok; Venkatraman, Srikanth; Parekh, Tejal N.; Gu, Haining; Njoroge, F. George; Girijavallabhan, Viyyoor M.; Ganguly, Ashit; Saksena, Anil; Jao, Edwin; Yao, Nanhua H.; Prongay, Andrew J.; Madison, Vincent S.; Vibulbhan, Banacha

PA Schering Corporation, USA

SO PCT Int. Appl., 402 pp.

CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2001077113	A2	20011018	WO 2001-US10869	20010403 <--
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	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
	CA 2405521	AA	20011018	CA 2001-2405521	20010403 <--
	AU 2001053124	A5	20011023	AU 2001-53124	20010403 <--
	US 2002107181	A1	20020808	US 2001-825399	20010403 <--
	US 6846802	B2	20050125		
	EP 1268525	A2	20030102	EP 2001-926601	20010403 <--
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				

BR 2001009861	A	20030610	BR 2001-9861	20010403
JP 2003530401	T2	20031014	JP 2001-575586	20010403
NZ 521455	A	20040625	NZ 2001-521455	20010403
ZA 2002007845	A	20040211	ZA 2002-7845	20020930
NO 2002004797	A	20021204	NO 2002-4797	20021004 <--
PRAI US 2000-194607P	P	20000405		
WO 2001-US10869	W	20010403		
OS MARPAT 135:318715				
GI				

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB Title compds. I [wherein X and Y = independently (cyclo)alkyl, heteroalkyl, (aryl)heteroaryl, alkyl(hetero)aryl, substituted ether, sulfide, sulfone, amide, sulfonamide, urea, carbamate, hydrazide, carbonyl, etc.; R1 = CHO, acyl, or (un)substituted carboxy, carbamoyl, boryl, etc.; Z = O, N, or CH, W = null or CO, CS, or SO<sub>2</sub>; Q = null or CH, N, P, (CH<sub>2</sub>)p, (CHR)p, (CRR')p, O, NR, S, or SO<sub>2</sub>; A = O, CH<sub>2</sub>, (CHR)p, (CHRCHR')p, (CRR')p, NR, S, SO<sub>2</sub>, or a bond; E = CH, N, CR, or a double bond toward A, L, or G; G = null or (CH<sub>2</sub>)p, (CHR)p, or (CRR')p; J = null or CH, CR, O, S, or NR; M = null or O, NR, S, SO<sub>2</sub>, "(CH<sub>2</sub>)p, (CHR)p, (CHRCHR')p, or (CRR')p; p = 0-6; R, R', R<sub>2</sub>, R<sub>3</sub>, and R<sub>4</sub> = independently H, (cyclo)alkyl, alkenyl, heterocycloalkyl, alkoxy, aryloxy, alkylthio, arylthio, amino, amido, ester, carboxylic acid, carbamate, urea, ketone, CHO, CN, NO<sub>2</sub>, O, N, S, P, etc.] were prepared as hepatitis C virus (HCV) protease inhibitors. For example, II (multi-step preparation given) was cyclized, deesterified, and coupled with III•HCl (preparation given) to give the macrocyclic hydroxyamide intermediate. Oxidation using Des-Martin reagent followed by flash chromatog. afforded two diastereomers IV in 82% combined yield. The (S)-isomer inhibited NS3-serine protease HeLa/Huh7 co-transfected cells with a K<sub>i</sub> of 2 μM. The invention also discloses pharmaceutical compns. comprising I as well as methods of using them to treat disorders associated with the HCV protease.

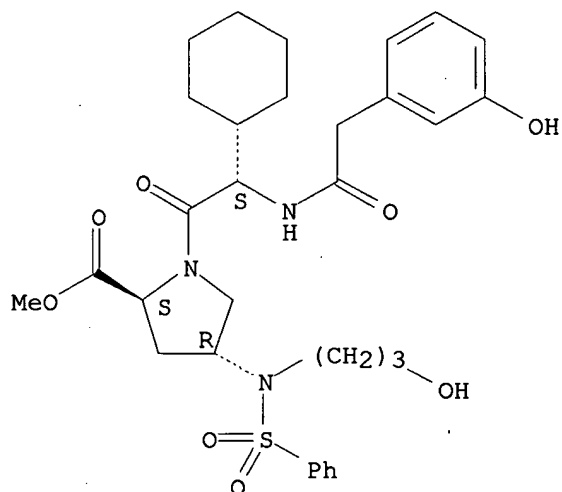
IT **367261-32-3**

RL: RCT (Reactant); RACT (Reactant or reagent)  
(preparation of macrocyclic NS3-serine protease inhibitors of hepatitis C virus comprising cyclic p2 moieties)

RN 367261-32-3 CAPLUS

CN L-Proline, (2S)-2-cyclohexyl-N-[(3-hydroxyphenyl)acetyl]glycyl-4-[(3-hydroxypropyl)(phenylsulfonyl)amino]-, methyl ester, (4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 367260-04-6P 367260-06-8P

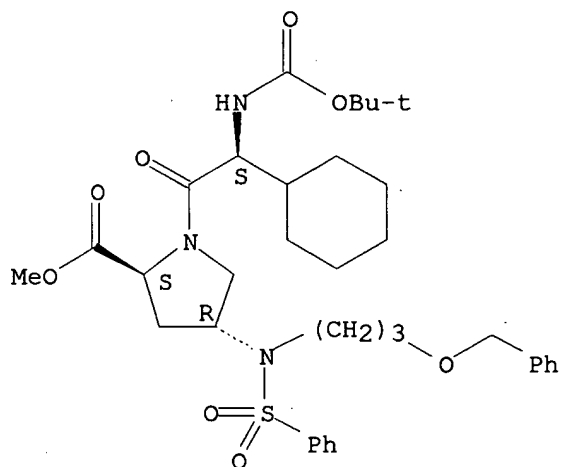
RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of macrocyclic NS3-serine protease inhibitors of hepatitis C virus comprising cyclic p2 moieties)

RN 367260-04-6 CAPLUS

CN L-Proline, (2S)-2-cyclohexyl-N-[(1,1-dimethylethoxy)carbonyl]glycyl-4-[[3-(phenylmethoxy)propyl](phenylsulfonyl)amino]-, methyl ester, (4R)- (9CI)  
(CA INDEX NAME)

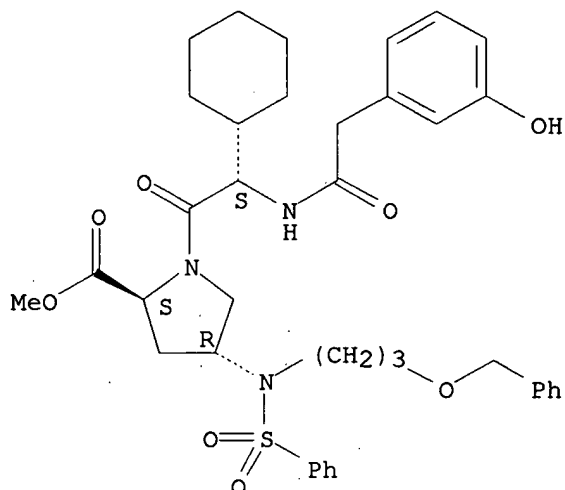
Absolute stereochemistry.



RN 367260-06-8 CAPLUS

CN L-Proline, (2S)-2-cyclohexyl-N-[(3-hydroxyphenyl)acetyl]glycyl-4-[[3-(phenylmethoxy)propyl](phenylsulfonyl)amino]-, methyl ester, (4R)- (9CI)  
(CA INDEX NAME)

Absolute stereochemistry.



=&gt; s 14 not 15

L6 3 L4 NOT L5

=&gt; dis 16 1-3 bib abs

L6 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2005 ACS on STN

AN 2005:451355 CAPLUS

DN 143:7980

TI Preparation of amino acid aminoheterocyclyl amides as melanocortin receptor agonists

IN Lee, Koo; Park, Heui-Sul; Ahn, In-Ae; Yoo, Hyun-Ju; Kim, Jong-Yup; Choi, Deog-Young; Yim, Hyeon-Joo; Chung, Kyung-Ha; Shim, Dong-Sup; Lee, Sang-Kyun; Kondoh, Yutaka; Hirabayashi, Ryoji; Honda, Shugo; Kaku, Hidetaka; Shishikura, Jun-ichi; Ito, Hiroyuki; Kurama, Takeshi

PA Lg Life Sciences Ltd., S. Korea; Yamanouchi Pharmaceutical Co., Ltd.

SO PCT Int. Appl., 117 pp.

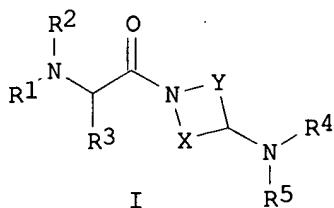
CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2005047251	A1	20050526	WO 2004-KR2929	20041112
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PRAI KR 2003-79799	A	20031112		
KR 2004-65820	A	20040820		
GI				



AB The invention relates to amino acid derivs. I [X, Y = CH<sub>2</sub> or CH<sub>2</sub>CH<sub>2</sub>; R<sub>1</sub> = H, (CH<sub>2</sub>)<sub>0-3</sub>-R<sub>6</sub>, (CH<sub>2</sub>)<sub>0-3</sub>CO(CH<sub>2</sub>)<sub>0-3</sub>-R<sub>6</sub>, (CH<sub>2</sub>)<sub>0-3</sub>SO<sub>2</sub>(CH<sub>2</sub>)<sub>0-3</sub>-R<sub>6</sub>, etc., where R<sub>6</sub> = (un)substituted alkyl, alkoxy, cycloalkyl, heterocyclyl, aryl, heteroaryl, amino or hydroxy; R<sub>2</sub> = H, (un)substituted alkyl, cycloalkyl or CO(CH<sub>2</sub>)<sub>0-3</sub>-R<sub>6</sub>; R<sub>3</sub>, R<sub>4</sub> = H, alkyl, (CH<sub>2</sub>)<sub>0-3</sub>-cycloalkyl, -aryl, -heteroaryl or -heterocyclyl in which the rings may be substituted; R<sub>5</sub> = H, alkyl, or (CH<sub>2</sub>)<sub>0-3</sub> substituted by acyl, (thio)carbamoyl, sulfamoyl or sulfonyl groups; or R<sub>1</sub>R<sub>2</sub>N, R<sub>4</sub>R<sub>5</sub>N = heterocyclyl], including pharmaceutically-acceptable salts, hydrates, solvates and isomers, which are effective agonists of the melanocortin receptor (MCR). Thus, (2R)-2-amino-N-[(3S)-3-(cyclohexyl(isobutyryl)amino)pyrrolidine-1-yl]-3-(4-chlorophenyl)propionamide TFA salt was prepared via amidation reaction and showed EC<sub>50</sub> = 0.005-0.5 μM and IC<sub>50</sub> = 0.1-0.5 μM against MCR4.

RE.CNT 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2005 ACS on STN

AN 2004:964812 CAPLUS

DN 141:411215

TI Preparation of amino acid heterocyclyl amides as modulators of the melanocortin-4 receptor

IN Chaturvedula, Prasad V.; Luo, Guanglin; Vig, Shikha; Poindexter, Graham S.; Beno, Brett R.

PA USA

SO U.S. Pat. Appl. Publ., 31 pp.

CODEN: USXXCO

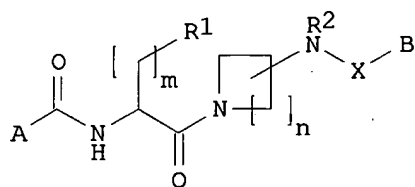
DT Patent

LA English

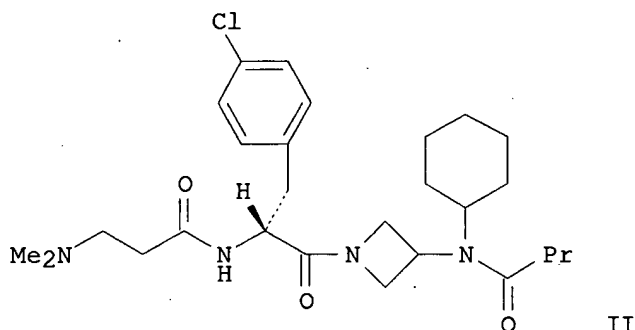
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 2004224901	A1	20041111	US 2004-813870	20040330
PRAI	US 2003-465552P	P	20030425		
OS	MARPAT 141:411215				
GI					





I



II

AB Novel azetidiny and pyrrolidinyl compds. I [A is H, alkyl, aminoalkyl, optionally N-alkylated azetidiny, pyrrolidinyl, piperidinyl, piperazinyl, (thio)morpholinyl or (iso)quinolinyl; R1 is (un)substituted Ph, naphthyl, benzofuranyl, benzothienyl or indolyl; R2 is alkyl or cycloalkyl; m is 0-3; n is 1 or 2; X is CO or SO<sub>2</sub>; B is alkyl, cycloalkyl, cycloalkylmethyl, methoxy- or phenoxyalkyl, (un)substituted Ph, naphthyl, pyridinyl, pyrimidinyl, pyridazinyl, pyrazinyl, furanyl, thienyl, pyrrolyl, oxazolyl, isoxazolyl, benzfuranyl, benzthienyl, indolyl, benzoxazolyl or indazolyl] and their pharmaceutically-acceptable salts are ligands of melanocortin-4 receptors (MC4R) and are useful for treating conditions responsive to the modulation of melanocortin-4 receptors such as obesity, diabetes, and sexual dysfunction. Thus, 4-chlorophenylalanyl azetidine derivative II was prepared via acylation reactions and showed IC<sub>50</sub> < 250 nM in the MC4R binding assay.

L6 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2005 ACS on STN

AN 2004:370923 CAPLUS

DN 140:391302

TI Preparation of benzo-1,3-diazepin-2-ones and related compounds as CGRP receptor antagonists for the treatment of migraine headaches

IN Rudolf, Klaus; Mueller, Stephan Georg; Stenkamp, Dirk; Lustenberger, Philipp; Dreyer, Alexander; Bauer, Eckhart; Schindler, Marcus; Arndt, Kirsten; Doods, Henri

PA Boehringer Ingelheim, Germany

SO PCT Int. Appl., 254 pp.

CODEN: PIXXD2

DT Patent

LA German

FAN.CNT. 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2004037811	A1	20040506	WO 2003-EP11763	20031023
	WO 2004037811	C1	20050519		
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 LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ,  
 OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM,  
 TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW  
 RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,  
 KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES,  
 FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR,  
 BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG  
 DE 10250082 A1 20040513 DE 2002-10250082 20021025  
 US 2004132716 A1 20040708 US 2003-685921 20031015  
 PRAI DE 2002-10250082 A 20021025  
 US 2002-426167P P 20021114  
 OS MARPAT 140:391302  
 GI

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB Title compds. I [A = O, S, phenylsulfonylimino, etc.; X = O, S, substituted imino, etc.; Y, Z = alkyl, difluoromethyl, trifluoromethyl, etc.; R1 = 5-7 membered aza, diaza, triaza, etc. heterocycle; R2 = H, phenylmethyl, alkyl, etc.; R3 = H, Ph, pyridinyl, etc.] and their pharmaceutically acceptable salts and formulations were prepared For example, benzo-1,3-diazepin-2-one II was prepared from 1-(3,4-diethylphenyl)ethanone in 8-steps. In human CGRP receptor binding affinity assays, compds. I exhibited IC50 values < 10000 nM. Compds. I are claimed useful for the treatment of migraine headaches.

RE.CNT 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD  
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> log y

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
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FULL ESTIMATED COST	20.62	183.02
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
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CA SUBSCRIBER PRICE	-3.65	-3.65

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